

# Multi-band Wigner Function Formulation of Quantum Transport

Mehmet Burcin Unlu, Bernard Rosen, and Hong-Liang Cui

*Department of Physics and Engineering Physics, Stevens Institute of Technology,  
Hoboken, New Jersey 07030*

Peiji Zhao

*Department of Electrical and Computer Engineering, North Carolina State  
University, Raleigh, North Carolina 27695*

## Abstract

A Wigner function representation of multi-band quantum transport theory is developed in this paper. The equations are derived using non-equilibrium Green's function formulation with the generalized Kadanoff-Baym ansatz and the multi-band  $\mathbf{k} \cdot \mathbf{p}$  Hamiltonian including spin. The results are applied to a two-band resonant inter-band tunneling structure.

*Key words:* Wigner function equation, Multi-band semiconductor systems

*PACS:* 72.10.-d, 79.60.Jv

## 1 Introduction

The single band approximation [2] is the most often used approach in quantum device models. In this approximation, inter-band processes in the structure are ignored and the boundary conditions for the model are oversimplified. The single band electron transport models have been applied to large band-gap semiconductor heterostructures (e.g. AlAs/GaAs/AlAs).

Multi-band quantum transport has attracted attention due to the existence of various inter-band tunneling structures and especially resonant inter-band tunneling structures (RITS). It is possible to achieve multiple negative differential regions (NDR) in these structures and they are shown to exhibit high peak-to-valley current voltage characteristics. RITS's are based upon the type-I, the type-II staggered and the type-II broken-gap band alignments. Recently

[3], it was theoretically shown that a type-II staggered band-gap resonant tunneling diode can exhibit oscillations in the THz region. A significant amount of inter-band current can be present in a staggered band-gap structure. The coupling between the conduction and the valence bands is considered to be the dominant mechanism in these structures. Therefore, in a correct description of electron transport, multi-band effects must be included [4]. We do not consider an external magnetic field but the extension is quite straightforward.

For direct band-gap semiconductors the conduction band near  $k = 0$  has symmetry properties (spherical symmetry) same as the  $|S\rangle$  atomic orbital ( $l = 0, m_l = 0$ ). On the other hand, the valence band near  $k = 0$  has symmetry of p-orbitals,  $|X\rangle, |Y\rangle$  and  $|Z\rangle$  (p-orbitals are antisymmetric and  $l = 1, m_l = -1, 0, 1$ ). An eight-band model [5] can be gained with the inclusion of spin. These states that become doubly degenerate,  $|S\uparrow\rangle, |X\uparrow\rangle, |Y\uparrow\rangle, |Z\uparrow\rangle, |S\downarrow\rangle, |X\downarrow\rangle, |Y\downarrow\rangle, |Z\downarrow\rangle$ . The spin-orbit interaction lifts the six-fold degeneracy of the valence band and splits it into a four-fold degenerate and a two-fold degenerate level. If the spin-orbit coupling is considered in the energy band calculation of a semiconductor, the Bloch states become a mixture of spin up and spin down states. This becomes important in asymmetric quantum well devices. Inversion asymmetry of the bulk or the confining potential causes spin splitting even in zero magnetic field due to spin-orbit interaction. Therefore inclusion of spin and spin-orbit interaction in the quantum transport equations is important.

Derivations of quantum transport equations have usually been based on the first-order gradient expansion [6]. This approximation is based on the assumption that the “fast” quantum variations can be separated from the “slow” macroscopic variations and causes the loss of information related to quantum processes such as interference and tunneling which are crucial in nano-scale devices. Buot and Jensen [2], [7] presented an alternative derivation for single-band devices and provided an exact integral form of the quantum transport equation which is capable of accurately describing full quantum effects. The first-order gradient expansion is still needed to simplify the collision terms after the derivation of transport equations. Their approach has been generalized for the multi-band transport in this work.

The Wigner function modeling of the quantum transport in the single-band resonant tunneling structures has been quite popular in the literature due to its success in dealing with the dissipation and the open boundary conditions [2]. Similarly, it is expected that one should be able to model the multi-band transport in the resonant tunneling structures using the Wigner function.

There are a number of works on multi-band Wigner function representation of quantum transport in the literature. Miller and Neikirk [8] used Wigner function for multi-subband transport in double barrier resonant tunneling struc-

tures. Demei et al. presented multi-band Wigner function formulation without spin [9], [10]. Zhao et al. [11] showed that multi-band quantum transport equations can be decoupled to reduce the number equations to be solved. Borgioli [12] employed a two-band Kane model to derive Wigner function equations for resonant inter-band tunneling diodes.

The point of this work is to develop a complete theory of the multi-band Wigner function for transport in nano-scale devices. This has been accomplished by using non-equilibrium Green's function methodology which is known to be the most complete description of quantum transport. The results give us the Wigner function formulation of multi-band systems based on  $\mathbf{k} \cdot \mathbf{p}$  theory. The results can be easily simplified by the symmetry arguments of the band structure of the system under study. The derived multi-band Wigner function equations which are also capable of description of zero magnetic field spin transport devices are the first in the literature.

In the introduction, the subsection 1.1 we present a preliminary on  $\mathbf{k} \cdot \mathbf{p}$  method. Then in the subsection 1.2, the non-equilibrium Green's function method in phase space is given. We derive the Wigner function equations for multi-band systems in section 2. Finally, in part section 3, we apply the formalism to a simple one dimensional two-band resonant inter-band tunneling diode.

### 1.1 $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian

The Schrödinger equation for the lattice periodic part of the Bloch functions can be written as [13]

$$\left[ \frac{\hat{p}^2}{2m_0} + V(\mathbf{r}) + \frac{\hbar^2 k^2}{2m_0} + \frac{\hbar}{m_0} \mathbf{k} \cdot \hat{\mathbf{p}} + \frac{\hbar^2}{4m_0^2 c^2} (\hat{\sigma} \times \nabla V) \cdot \hat{\mathbf{p}} + \frac{\hbar}{4m_0^2 c^2} (\hat{\sigma} \times \nabla V) \cdot \mathbf{k} \right] |n\mathbf{k}\rangle = \varepsilon_{n\mathbf{k}} |n\mathbf{k}\rangle . \quad (1)$$

We express the bulk band matrix element  $H_{ab}$  of the Hamiltonian in the second order  $\mathbf{k} \cdot \mathbf{p}$  theory as

$$H_{ab} = D_{ab}^{(2)\alpha\gamma} k_\alpha k_\gamma + D_{ab}^{(1)\alpha} k_\alpha + (D_{aa}^{(0)} + V_a(\mathbf{r})) \delta_{ab} \quad (2)$$

where the indices  $\alpha$  and  $\gamma$  are summed over  $x$ ,  $y$ , and  $z$ . The  $a$ ,  $b$  include both the band and the spin indices.  $V(\mathbf{r})$  is a spin-independent self-consistent potential. Note that for heterostructures  $k_\alpha$  is replaced by  $-i\nabla_\alpha$ .

We define a vector  $\pi$  as,

$$\pi = \mathbf{p} + \frac{\hbar}{4m_0c^2}(\hat{\sigma} \times \nabla \mathbf{V}). \quad (3)$$

So,

$$D_{ab}^{(2)\alpha\gamma} = \frac{\hbar^2}{2m_0}\delta_{ab}\delta_{\alpha\gamma} + \left(\frac{\hbar}{m_0}\right)^2 \sum_r \frac{\pi_{ar}^\alpha \pi_{rb}^\gamma}{\left(\frac{E_a+E_b}{2} - E_r\right)}, \quad (4)$$

noting that the second term arises from Löwdin renormalization and needed to include the interactions with remote bands. So we denote these states by the index  $r$ . These interactions are usually ignored in Kane models and so  $D_{ab}^{(2)\alpha\gamma}(a \neq b)$  terms vanish.

The part of  $H_{ab}$  linear in  $k$  include the inter-band coupling ( $\mathbf{k} \cdot \mathbf{p}$  interaction) and the spin-orbit interaction terms,

$$D_{ab}^{(1)\alpha} = \frac{\hbar}{m_0}\pi_{ab}^\alpha = \frac{\hbar}{m_0}p_{ab}^\alpha + \frac{\hbar}{4m_0^2c^2}(\hat{\sigma} \times \nabla V)_{ab}^\alpha \quad (5)$$

where

$$\pi_{ab}^\alpha = \langle U_a | \hat{p}^\alpha | U_b \rangle + \frac{1}{4m_0c^2} \langle U_a | (\hat{\sigma} \times \nabla V)^\alpha | U_b \rangle \quad (6)$$

for  $a \neq b$ . Note that  $\pi_{ba}^\alpha = (\pi_{ab}^\alpha)^*$  and  $\pi_{aa}^\alpha = 0$  (which implies that  $D_{aa}^{(1)\alpha}$  terms vanish).

The terms  $p_{ab}^\alpha = \langle U_a | \hat{p}^\alpha | U_b \rangle$  are the inter-band momentum matrix elements and measure the strength of the coupling between the various bands. Note that  $\pi_{aa}^\alpha = 0$  even if the band minimum is at some point other than  $\mathbf{k} = 0$ . The term  $\frac{\hbar}{m_0}p_{ab}^\alpha$  is usually written in terms of a real parameter  $P$  originally defined by Kane. The value of this parameter is known for any given material.

$$P = -\frac{i\hbar}{m_0} \langle S | \hat{p}_x | X \rangle = -\frac{i\hbar}{m_0} \langle S | \hat{p}_y | Y \rangle = -\frac{i\hbar}{m_0} \langle S | \hat{p}_z | Z \rangle. \quad (7)$$

The band edge is denoted by  $D_{aa}^{(0)}$  such that,  $D_{aa}^{(0)} = E_a(\mathbf{k} = 0)$ . We write  $D_{aa}^{(0)} + V_a(\mathbf{r})$  as  $E_a(\mathbf{r})$  in the calculations.

## 1.2 The non-equilibrium Green's function formalism in phase space

The multi-band Green's function [1] is defined by

$$G_{ab}(1, 2) = -\frac{i}{\hbar} \langle \psi_a(1) \psi_b^\dagger(2) \rangle_C \quad (8)$$

where C denotes that time arguments are on a contour rather than a real-time axis. The expectation value is defined in a grand-canonical ensemble. We define the space time arguments  $1 = (\mathbf{r}_1, \mathbf{t}_1)$ ,  $2 = (\mathbf{r}_2, \mathbf{t}_2)$ .  $\psi_a$  is the field operator for electrons. The  $a, b$  include both the band and the spin indices. The equation of motion of the band electron Green's function is written as (sum over repeated indices)

$$[i\hbar\delta_{a\beta}\frac{\partial}{\partial t_1} - H_{a\beta}(1)]G_{\beta b}(1, 2) = \delta_{ab}\delta(1 - 2) + \int d3\Sigma_{a\beta}(1, 3)G_{\beta b}(3, 2), \quad (9)$$

and the adjoint equation is given by

$$[-i\hbar\delta_{a\beta}\frac{\partial}{\partial t_2} - H_{a\beta}(2)]G_{\beta b}(1, 2) = \delta_{ab}\delta(1 - 2) + \int d3G_{a\beta}(1, 3)\Sigma_{\beta b}(3, 2), \quad (10)$$

where the self-energy is denoted by  $\Sigma(1, 2)$ . It describes the scattering of electrons by other electrons, phonons and impurities. Throughout the paper, Greek indices are used to denote the repeated indices to be summed over.

The generalized Kadanoff-Baym (GKB) equation describes the time evolution of the electron correlation function  $G_{aa}^<(1, 2)$  in the band  $a$ . It should be noted that, in the equal time limit ( $t_1 = t_2$ ), the off-diagonal ( $a \neq b$ ) lesser Green's functions correspond to inter-band polarizations in energy band space and inter-spin-band polarizations in spin space whereas the diagonal Green's functions give the particle densities with the spin up or down in each band. The time evolution of  $G^<(1, 2)$  given by the GKB equation can be written, using the Langreth algebra, as

$$\begin{aligned} i\hbar(\frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2})G_{ab}^<(1, 2) &= [H, G^<](1, 2)_{ab} + [\Sigma^<, \text{Re}G^R](1, 2)_{ab} \\ &\quad + \frac{i}{2}\{\Sigma^<, A\}(1, 2)_{ab} - \frac{i}{2}\{\Gamma, G^<\}(1, 2)_{ab}. \end{aligned} \quad (11)$$

where  $[ ]$  is the commutation and  $\{ \}$  is the anti-commutation. Above, the spectral function is defined as,

$$A_{ab}(1, 2) = i[G_{ab}^>(1, 2) - G_{ab}^<(1, 2)] = -2\text{Im}[G_{ab}^R(1, 2)], \quad (12)$$

and the dissipation function is

$$\Gamma_{ab}(1, 2) = i[\Sigma_{ab}^> - \Sigma_{ab}^<] = -2\text{Im}[\Sigma_{ab}^R(1, 2)]. \quad (13)$$

Switching to center of mass and relative coordinates (Wigner coordinates) done by defining

$$\mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}; T = \frac{t_1 + t_2}{2}, \quad (14)$$

$$\mathbf{v} = \mathbf{r}_2 - \mathbf{r}_1; t = t_2 - t_1. \quad (15)$$

The four-dimensional, (3+1), crystal momentum and its conjugate variable lattice coordinate are represented as  $p = (\mathbf{p}, E)$ ,  $r = (\mathbf{R}, T)$ . Note that we use  $\hbar\mathbf{k}$  as the crystal momentum when the matrix elements of the Hamiltonian is considered. Therefore  $\hbar\mathbf{k}$  and  $\mathbf{p}$  are used as the crystal momentum interchangeably.

The Weyl-Wigner representation,  $W[\hat{O}] = O(p, r)$ , of any operator  $\hat{O}(1, 2)$  [14], [15] is defined by

$$O(p, r) = \int dv \exp\left(\frac{i}{\hbar} p \cdot v\right) \langle R - \frac{v}{2} | \hat{O} | R + \frac{v}{2} \rangle. \quad (16)$$

It is very important to note that  $O(p, r)$  is real if  $\hat{O}$  is hermitian. Let  $\hat{C} = \hat{A}\hat{B}$  then the differential form of the Weyl transform of the product of two operators can be obtained by,

$$\begin{aligned} W[\hat{C}] &= C(p, r) = \exp(i\hat{\Lambda})\hat{A}(p, r)\hat{B}(p, r) \\ &= \exp(-i\hat{\Lambda})\hat{B}(p, r)\hat{A}(p, r), \end{aligned} \quad (17)$$

where

$$\hat{\Lambda} = \frac{\hbar}{2} \left[ \frac{\partial^{(A)}}{\partial r} \frac{\partial^{(B)}}{\partial p} - \frac{\partial^{(A)}}{\partial p} \frac{\partial^{(B)}}{\partial r} \right]. \quad (18)$$

The partial differential  $\partial^{(A)}$  acts on only  $A$  and  $\partial^{(B)}$  acts on  $B$  only.

To obtain the Wigner function equation, it is necessary to switch to a phase space description of GKB. Taking the Weyl-Wigner transform of both sides of the equation (11) gives the GKB in the phase-space-energy-time domain

$$i\hbar \frac{\partial}{\partial T} G_{ab}^<(p, r) = \exp(i\hat{\Lambda})[H, G^<](p, r)_{ab} + \exp(i\hat{\Lambda})[\Sigma^<, \text{Re}G^R](p, r)_{ab}$$

$$+\frac{i}{2}\exp(i\hat{\Lambda})\{\Sigma^<,A\}(p,r)_{ab}-\frac{i}{2}\exp(i\hat{\Lambda})\{\Gamma,G^<\}(p,r) \quad (19)$$

For any operator  $A$  and  $B$ , the integral representations of  $\exp(i\hat{\Lambda})A(p,r)B(p,r)$  and  $\exp(-i\hat{\Lambda})A(p,r)B(p,r)$  in (3+1) dimensions can be written as [1],

$$\begin{aligned} \exp(\pm i\hat{\Lambda})A(p,r)B(p,r) &= \frac{1}{(h^4)^2} \int dr_1 dp_1 dr_2 dp_2 \exp\left[\frac{i}{\hbar} p_1 \cdot (r - r_2)\right] \exp\left[\frac{i}{\hbar} r_1 \cdot (p - p_2)\right] \\ &\quad \times A(p \pm \frac{p_1}{2}, r \mp \frac{r_1}{2}) B(p_2, r_2), \end{aligned} \quad (20)$$

Defining

$$K_A^\pm(p, r - r_2; r, p - p_2) = \int dp_1 dr_1 \exp\left(\frac{i}{\hbar} p_1 \cdot (r - r_2)\right) \exp\left(\frac{i}{\hbar} r_1 \cdot (p - p_2)\right) A(p \pm \frac{p_1}{2}, r \mp \frac{r_1}{2}), \quad (21)$$

the equation (19) becomes

$$\begin{aligned} i\hbar \frac{\partial}{\partial T} G_{ab}^<(p, r) &= \frac{1}{(h^4)^2} \int dp_2 dr_2 K_{H_{a\beta}}^c(p, r - r_2; r, p - p_2) G_{\beta b}^<(p_2, r_2) \\ &\quad + \frac{1}{(h^4)^2} \int dp_2 dr_2 K_{\Sigma_{a\beta}^<}^c(p, r - r_2; r, p - p_2) \text{Re}G_{\beta b}^R(p_2, r_2) \\ &\quad + \frac{i}{2(h^4)^2} \int dp_2 dr_2 K_{\Sigma_{a\beta}^<}^s(p, r - r_2; q, p - p_2) A_{\beta b}(p_2, r_2) \\ &\quad - \frac{i}{2(h^4)^2} \int dp_2 dr_2 K_{\Gamma_{a\beta}}^s(p, r - r_2; r, p - p_2) G_{\beta b}^<(p_2, r_2) \end{aligned} \quad (22)$$

where  $K_A^{s,c}(p, r - r_2; r, p - p_2) = K_A^+(p, r - r_2; r, p - p_2) \pm K_A^-(p, r - r_2; r, p - p_2)$ .

The multi-band Wigner function is found by taking the energy integral of the Weyl-Wigner transformed  $G_{ab}^<$ :

$$f_{ab}(\mathbf{p}, \mathbf{R}, T) = \int dE (-i) G_{ab}^<(\mathbf{p}, E; \mathbf{R}, T). \quad (23)$$

Note that the indices  $a, b$  include both spin and band. The total Wigner function of the multi-band system with spin can be written as the summation over the band and the spin indices,

$$f(\mathbf{p}, \mathbf{r}, \kappa) = \sum_{c,d} \sum_{m,m'=\uparrow,\downarrow} \sigma_{m,m'}^\kappa f_{cd}^{mm'}(\mathbf{p}, \mathbf{r}), \quad (24)$$

where  $c, d$  are band,  $m$  and  $m'$  are spin indices.  $\kappa$  takes values of  $x, y$ , and  $z$ .  $\sigma^0$  is the unit matrix and the others are the Pauli spin matrices [16]. Therefore

each intra-band and inter-band component of Wigner function becomes  $2 \times 2$  matrix in spin space.

## 2 The Wigner Function Equations for Multi-band Systems

Under the assumption that the self-energies are slowly varying with respect to the center of mass coordinates, equation (22) reduces to

$$\begin{aligned} i\hbar \frac{\partial}{\partial T} G_{ab}^<(p, r) = & \frac{1}{(h^4)^2} \int dp_2 dr_2 K_{H_{a\beta}}^c(p, r - r_2; r, p - p_2) G_{\beta b}^<(p_2, r_2) \\ & + \Sigma_{a\beta}^>(p, r) G_{\beta b}^<(p, r) - \Sigma_{a\beta}^<(p, r) G_{\beta b}^>(p, r) \end{aligned} \quad (25)$$

using

$$i[\Sigma_{a\beta}^< A_{\beta b} - \Gamma_{a\beta} G_{\beta b}^<] = \Sigma_{a\beta}^> G_{\beta b}^< - \Sigma_{a\beta}^< G_{\beta b}^>. \quad (26)$$

The self-energy function can be written as [17],

$$\Sigma_{ab}^{>,<}(1, 2) = iG_{ab}^{>,<}(1, 2)D^{>,<}(1, 2). \quad (27)$$

The Weyl-Wigner transform gives of the above equation (27) gives,

$$\Sigma_{ab}^{>,<}(p, r) = \frac{i}{h^4} \int dq G_{ab}^{>,<}(p + q) D^{>,<}(q). \quad (28)$$

Assuming the phonon bath is in equilibrium, the Fourier transforms of the phonon Green's functions can be written as,

$$D^<(\mathbf{q}, E') = -ihM_{\mathbf{q}}^2[(N_{\mathbf{q}} + 1)\delta(E' - \Omega_{\mathbf{q}}) + N_{\mathbf{q}}\delta(E' + \Omega_{\mathbf{q}})], \quad (29)$$

$$D^>(\mathbf{q}, E') = -ihM_{\mathbf{q}}^2[(N_{\mathbf{q}} + 1)\delta(E' + \Omega_{\mathbf{q}}) + N_{\mathbf{q}}\delta(E' - \Omega_{\mathbf{q}})] \quad (30)$$

where  $M_{\mathbf{q}}$  is the electron-phonon scattering matrix element. Therefore, inclusion of the phonon scattering gives the following scattering functions

$$\Sigma_{ab}^< = \sum_{\eta=+1,-1} \frac{1}{h^3} \int d\mathbf{q} G_{ab}^<(\mathbf{p} + \mathbf{q}, E + \eta\Omega_{\mathbf{q}}, r) M_{\mathbf{q}}^2(N_{\mathbf{q}} + \frac{1}{2} + \frac{1}{2}\eta), \quad (31)$$

$$\Sigma_{ab}^> = \sum_{\eta=+1,-1} \frac{1}{h^3} \int d\mathbf{q} G_{ab}^>(\mathbf{p} + \mathbf{q}, E + \eta\Omega_{\mathbf{q}}, r) M_{\mathbf{q}}^2(N_{\mathbf{q}} + \frac{1}{2} - \frac{1}{2}\eta). \quad (32)$$

The first term on the right hand side of the equation (25) can be written as

$$\exp(i\Lambda)[H, G^<](p, r)_{ab} = \exp(i\Lambda)H_{a\beta}(p, r)G_{\beta b}^<(p, r) - \exp(-i\Lambda)H_{\beta b}(p, r)G_{a\beta}^<(p, r). \quad (33)$$

The integral representation, using the equation (20) becomes

$$\begin{aligned} \exp(i\Lambda)[H, G^<](p, r)_{ab} &= \frac{1}{(h^4)^2} \int dr_1 dp_1 dr_2 dp_2 \exp\left(\frac{i}{\hbar}p_1 \cdot (r - r_2)\right) \exp\left(\frac{i}{\hbar}r_1 \cdot (p - p_2)\right) \\ &\quad \times [H_{a\beta}\left(\mathbf{p} + \frac{\mathbf{p}_1}{2}, \mathbf{q} - \frac{\mathbf{q}_1}{2}\right)G_{\beta b}^<(p_2, q_2) \\ &\quad - H_{\beta b}\left(\mathbf{p} - \frac{\mathbf{p}_1}{2}, \mathbf{r} + \frac{\mathbf{r}_1}{2}\right)G_{a\beta}^<(p_2, r_2)], \end{aligned} \quad (34)$$

where

$$\begin{aligned} H_{ab}(p \pm \frac{p_1}{2}, r \mp \frac{r_1}{2}) &= D_{ab}^{(2)\alpha\gamma}(p_\alpha \pm \frac{p_{1\alpha}}{2})(p_\gamma \pm \frac{p_{1\gamma}}{2}) \\ &\quad + D_{ab}^{(1)\alpha}(p_\alpha \pm \frac{p_{1\alpha}}{2}) + (D_{aa}^{(0)} + V_a(\mathbf{r} \mp \frac{\mathbf{r}_1}{2}))\delta_{ab}. \end{aligned} \quad (35)$$

At this point, since the purpose of the paper is to derive a Boltzmann type transport equation, it is useful to make quasiparticle approximation to get the form of the spectral function. The free generalized Kadanoff-Baym (FGKB) ansatz for multi-band systems is stated as [18],

$$-iG_{ab}^<(\mathbf{p}, E, \mathbf{r}, T) = h f_{ab}(\mathbf{p}, \mathbf{r}, T) \delta(E - \frac{E_a(\mathbf{p}) + E_b(\mathbf{p})}{2}) \quad (36)$$

$$iG_{ab}^>(\mathbf{p}, E, \mathbf{r}, T) = h(\delta_{ab} - f_{ab}(\mathbf{p}, \mathbf{r}, T)) \delta(E - \frac{E_a(\mathbf{p}) + E_b(\mathbf{p})}{2}) \quad (37)$$

Using FGKB ansatz, one can simplify the scattering functions so that the equation of motion for  $G^<$  in the phase-space-energy-time domain becomes

$$\begin{aligned} i\hbar \frac{\partial}{\partial T} G_{ab}^<(\mathbf{p}, E, \mathbf{r}, T) &= D_{a\beta}^{(2)\alpha\gamma} p_\alpha p_\gamma G_{\beta b}^< - D_{\beta b}^{(2)\alpha\gamma} p_\alpha p_\gamma G_{a\beta}^< \\ &\quad + \frac{\hbar}{2i} D_{a\beta}^{(2)\alpha\gamma} [p_\alpha \frac{\partial}{\partial r_\gamma} + p_\gamma \frac{\partial}{\partial r_\alpha}] G_{\beta b}^< + \frac{\hbar}{2i} D_{\beta b}^{(2)\alpha\gamma} [p_\alpha \frac{\partial}{\partial r_\gamma} + p_\gamma \frac{\partial}{\partial r_\alpha}] G_{a\beta}^< \\ &\quad - \frac{\hbar^2}{4} D_{a\beta}^{(2)\alpha\gamma} \frac{\partial}{\partial r_\alpha} \frac{\partial}{\partial r_\gamma} G_{\beta b}^< + \frac{\hbar^2}{4} D_{\beta b}^{(2)\alpha\gamma} \frac{\partial}{\partial r_\alpha} \frac{\partial}{\partial r_\gamma} G_{a\beta}^< \\ &\quad + D_{a\beta}^{(1)\alpha} [p_\alpha + \frac{\hbar}{2i} \frac{\partial}{\partial r_\alpha}] G_{\beta b}^< - D_{\beta b}^{(1)\alpha} [p_\alpha - \frac{\hbar}{2i} \frac{\partial}{\partial r_\alpha}] G_{a\beta}^< \\ &\quad + \delta_{ab} \frac{1}{h^3} \int dp_2 dr_1 \exp\left(\frac{i}{\hbar}r_1 \cdot (p - p_2)\right) [D_{aa}^{(0)} + V_{aa}(\mathbf{r} - \frac{\mathbf{r}_1}{2})] G_{\beta b}^<(p_2, r) \end{aligned}$$

$$\begin{aligned}
& -\delta_{\beta b} \frac{1}{\hbar^3} \int dp_2 dr_1 \exp\left(\frac{i}{\hbar} r_1 \cdot (p - p_2)\right) [D_{\beta\beta}^{(0)} + V_{\beta\beta}(\mathbf{r} + \frac{\mathbf{r}_1}{2})] G_{a\beta}^<(p_2, r) \\
& + [\Sigma_{a\beta}^> G_{\beta b}^< - \Sigma_{a\beta}^< G_{\beta b}^>]
\end{aligned} \tag{38}$$

where  $p_\alpha$  denotes  $p_x, p_y, p_z$ ,  $\frac{\partial}{\partial r_\alpha}$  denotes  $\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}$  and there is summation over Greek indices as usual. Using the equation (23), the multi-band Wigner functions for an open system in weakly contact with a phonon heat bath can be written as

$$\begin{aligned}
i\hbar \frac{\partial}{\partial T} f_{ab}(\mathbf{p}, \mathbf{r}, T) = & D_{a\beta}^{(2)\alpha\gamma} p_\alpha p_\gamma f_{\beta b}(\mathbf{p}, \mathbf{r}, T) - D_{\beta b}^{(2)\alpha\gamma} p_\alpha p_\gamma f_{a\beta}(\mathbf{p}, \mathbf{r}, T) \\
& + \frac{\hbar}{2i} D_{a\beta}^{(2)\alpha\gamma} [p_\alpha \frac{\partial}{\partial r_\gamma} + p_\gamma \frac{\partial}{\partial r_\alpha}] f_{\beta b}(\mathbf{p}, \mathbf{r}, T) \\
& + \frac{\hbar}{2i} D_{\beta b}^{(2)\alpha\gamma} [p_\alpha \frac{\partial}{\partial r_\gamma} + p_\gamma \frac{\partial}{\partial r_\alpha}] f_{a\beta}(\mathbf{p}, \mathbf{r}, T) \\
& - \frac{\hbar^2}{4} D_{a\beta}^{(2)\alpha\gamma} \frac{\partial}{\partial r_\alpha} \frac{\partial}{\partial r_\gamma} f_{\beta b}(\mathbf{p}, \mathbf{r}, T) + \frac{\hbar^2}{4} D_{\beta b}^{(2)\alpha\gamma} \frac{\partial}{\partial r_\alpha} \frac{\partial}{\partial r_\gamma} f_{a\beta}(\mathbf{p}, \mathbf{r}, T) \\
& + D_{a\beta}^{(1)\alpha} [p_\alpha + \frac{\hbar}{2i} \frac{\partial}{\partial r_\alpha}] f_{\beta b}(\mathbf{p}, \mathbf{r}, T) - D_{\beta b}^{(1)\alpha} [p_\alpha - \frac{\hbar}{2i} \frac{\partial}{\partial r_\alpha}] f_{a\beta}(\mathbf{p}, \mathbf{r}, T) \\
& + \delta_{a\beta} \frac{1}{\hbar^3} \int dp_2 dr_1 \exp\left(\frac{i}{\hbar} r_1 \cdot (p - p_2)\right) [D_{aa}^{(0)} + V_{aa}(\mathbf{r} - \frac{\mathbf{r}_1}{2})] f_{\beta b}(\mathbf{p}, \mathbf{r}, T) \\
& - \delta_{\beta b} \frac{1}{\hbar^3} \int dp_2 dr_1 \exp\left(\frac{i}{\hbar} r_1 \cdot (p - p_2)\right) [D_{\beta\beta}^{(0)} + V_{\beta\beta}(\mathbf{r} + \frac{\mathbf{r}_1}{2})] f_{a\beta}(\mathbf{p}, \mathbf{r}, T) \\
& + \sum_{\eta=+1,-1} \frac{1}{\hbar^3} \int d\mathbf{q} (\delta_{a\beta} - f_{a\beta}(\mathbf{p} + \mathbf{q}, \mathbf{r}, T)) f_{\beta b}(\mathbf{p}, \mathbf{r}, T) \\
& \times \delta\left(\frac{E_a(\mathbf{p} + \mathbf{q}) + E_\beta(\mathbf{p} + \mathbf{q})}{2} - \frac{E_\beta(\mathbf{p}) + E_b(\mathbf{p})}{2} + \eta \Omega_{\mathbf{q}}\right) M_{\mathbf{q}}^2 (N_{\mathbf{q}} + \frac{1}{2} - \frac{1}{2}\eta) \\
& - \sum_{\eta=+1,-1} \frac{1}{\hbar^3} \int d\mathbf{q} f_{a\beta}(\mathbf{p} + \mathbf{q}, \mathbf{r}, T) (\delta_{\beta b} - f_{\beta b}(\mathbf{p}, \mathbf{r}, T)) \\
& \times \delta\left(\frac{E_a(\mathbf{p} + \mathbf{q}) + E_\beta(\mathbf{p} + \mathbf{q})}{2} - \frac{E_\beta(\mathbf{p}) + E_b(\mathbf{p})}{2} + \eta \Omega_{\mathbf{q}}\right) M_{\mathbf{q}}^2 (N_{\mathbf{q}} + \frac{1}{2} + \frac{1}{2}\eta)
\end{aligned} \tag{39}$$

The third and the fourth terms at the right of the equation (39) are the usual drift terms. The first, the second, the fifth and the sixth terms do not cancel each other for  $a \neq b$  if and only if Löwdin renormalization is considered. If the effects of the remote bands are ignored, these terms cancel each other. The seventh and eighth terms explicitly give the  $\mathbf{k} \cdot \mathbf{p}$  and spin-orbit interactions. The ninth and tenth terms give the potential term. The last two terms correspond to electron-phonon scattering. The relaxation time approximation can be made for these. An important simplification occurs when the in-plane wave vector is taken to be zero. This approximation gives a set of spin-independent quantum transport equations.

If the structure under consideration has inversion symmetry as in diamond structures, the equations can be simplified further. Note that there is no inversion symmetry in zinc-blende structures (bulk inversion asymmetry) and spin degeneracy in zinc-blende type heterostructures is lifted even at zero magnetic field. Usually, this splitting is very small and can be ignored. However, recently resonant intra-band and inter-band spin filter was proposed based on the zero magnetic field spin splitting of the conduction band in the case of structural inversion asymmetry (Rashba effect) [19], [20]. We are going to discuss the Wigner function modeling of these kind of devices in future papers.

The total current density is the sum of intra-band and inter-band components [14],

$$J(r) = \frac{q}{h^3} \int d\mathbf{p} \frac{\partial H_{\alpha\beta}}{\partial \mathbf{p}} f_{\beta\alpha}(\mathbf{p}, r). \quad (40)$$

The particle density in each band is written as

$$n_a = \frac{1}{h^3} \int d\mathbf{p} f_{aa}(\mathbf{p}, r). \quad (41)$$

Let's consider a two-band model ( $a, b = 1, 2$ ) without scattering and neglect the effects of the remote bands. Then the first component of the Wigner equation (39) becomes

$$\begin{aligned} i\hbar \frac{\partial f_{11}(\mathbf{p}, r)}{\partial T} &= \frac{\hbar}{i} D_{11}^{(2)\alpha\gamma} [p_\alpha \frac{\partial}{\partial r_\gamma} + p_\gamma \frac{\partial}{\partial r_\alpha}] f_{11}(\mathbf{p}, r) \\ &\quad + D_{12}^{(1)\alpha\gamma} [p_\alpha + \frac{\hbar}{2i} \frac{\partial}{\partial r_\alpha}] f_{21}(\mathbf{p}, r) - D_{21}^{(1)\alpha\gamma} [p_\alpha - \frac{\hbar}{2i} \frac{\partial}{\partial r_\alpha}] f_{12}(\mathbf{p}, r) \\ &\quad + \frac{1}{h^3} \int dp_2 dr_1 \exp(\frac{i}{\hbar} r_1 \cdot (p - p_2)) \\ &\quad \times [V_1(\mathbf{r} - \frac{\mathbf{r}_1}{2}) - V_1(\mathbf{r} + \frac{\mathbf{r}_1}{2})] f_{11}(\mathbf{p}_2, r). \end{aligned} \quad (42)$$

The rest of the equations are as follows

$$\begin{aligned} i\hbar \frac{\partial f_{12}(\mathbf{p}, r)}{\partial T} &= \frac{\hbar}{2i} [D_{11}^{(2)\alpha\gamma} + D_{22}^{(2)\alpha\gamma}] [p_\alpha \frac{\partial}{\partial r_\gamma} + p_\gamma \frac{\partial}{\partial r_\alpha}] f_{12}(\mathbf{p}, r) \\ &\quad + D_{12}^{(1)\alpha} [p_\alpha + \frac{\hbar}{2i} \frac{\partial}{\partial r_\alpha}] f_{22}(\mathbf{p}, r) - D_{12}^{(1)\alpha} [p_\alpha - \frac{\hbar}{2i} \frac{\partial}{\partial r_\alpha}] f_{11}(\mathbf{p}, r) \\ &\quad + \frac{1}{h^3} \int dp_2 dr_1 \exp(\frac{i}{\hbar} r_1 \cdot (p - p_2)) \\ &\quad \times [V_1(\mathbf{r} - \frac{\mathbf{r}_1}{2}) - V_2(\mathbf{r} + \frac{\mathbf{r}_1}{2})] f_{12}(\mathbf{p}_2, r), \end{aligned} \quad (43)$$

$$\begin{aligned}
i\hbar \frac{\partial f_{22}(\mathbf{p}, \mathbf{r}, T)}{\partial T} = & \frac{\hbar}{i} D_{22}^{(2)\alpha\gamma} [p_\alpha \frac{\partial}{\partial r_\gamma} + p_\gamma \frac{\partial}{\partial r_\alpha}] f_{22}(\mathbf{p}, r) \\
& + D_{21}^{(1)\alpha\gamma} [p_\alpha + \frac{\hbar}{2i} \frac{\partial}{\partial r_\alpha}] f_{12}(\mathbf{p}, r) - D_{12}^{(1)\alpha\gamma} [p_\alpha - \frac{\hbar}{2i} \frac{\partial}{\partial r_\alpha}] f_{21}(\mathbf{p}, r) \\
& + \frac{1}{h^3} \int dp_2 dr_1 \exp(\frac{i}{\hbar} r_1 \cdot (p - p_2)) \\
& \times [V_2(\mathbf{r} - \frac{\mathbf{r}_1}{2}) - V_2(\mathbf{r} + \frac{\mathbf{r}_1}{2})] f_{22}(\mathbf{p}_2, r),
\end{aligned} \tag{44}$$

and  $f_{21} = f_{12}^*$ .

### 3 1-Dimensional Two-band Kane Model of Resonant Inter-band Tunneling Diode

Resonant inter-band tunneling structures (RITS) are based on the interaction between the conduction and valence bands and the transport is in the growth direction. For narrow band-gap RIT structures, the coupling of the in-plane momentum to the transverse momentum component becomes important. Therefore a realistic modeling of these structures requires a serious amount of computational work.

The simplest choice is a two-band model that is suitable for large and mid-band-gap Type I RITS [21]. The  $\mathbf{k}$  vector is taken in the  $z$  direction and the inversion asymmetry is neglected. Therefore, the in-plane momentum ( $k_x = k_y = 0$ ) vanishes so that the heavy-hole state is decoupled and the Hamiltonian matrix becomes block-diagonal [22]. The remote bands are neglected too. Therefore the Hamiltonian is reduced to a spin-independent three-band model (conduction, light and split-off bands) [23]:

$$\begin{bmatrix} E_c(z) + \frac{p_z^2}{2m_0} & \sqrt{\frac{2}{3}} \frac{P_{cv}}{m_0} p_z & -\sqrt{\frac{1}{3}} \frac{P_{cv}}{m_0} p_z \\ -\sqrt{\frac{2}{3}} \frac{P_{cv}}{m_0} p_z & E_{lh}(z) + \frac{p_z^2}{2m_0} & 0 \\ \sqrt{\frac{1}{3}} \frac{P_{cv}}{m_0} p_z & 0 & E_{so}(z) + \frac{p_z^2}{2m_0} \end{bmatrix}. \tag{45}$$

where  $P_{cv} = i\sqrt{\frac{m_0 E_p}{2}}$ . Instead of ignoring the split-off band, Sirtori et. al. [23] presented an improved two-band model (conduction and “effective valence band”) that can be gained through a unitary transformation. The  $2 \times 2$  Hamiltonian is

$$\begin{bmatrix} E_c(z) + \frac{p_z^2}{2m_0} & \frac{P_{cv}}{m_0} p_z \\ \frac{P_{cv}^*}{m_0} p_z & E_v(z) + \frac{p_z^2}{2m_0} \end{bmatrix} \tag{46}$$

where  $E_v = \frac{2E_{lh} + E_{so}}{3}$  is effective valence band edge. Therefore the components of the Wigner function become

$$\begin{aligned} i\hbar \frac{\partial f_{cc}(p_z, z, t)}{\partial t} = & -\frac{i\hbar p_z}{m_0} \frac{\partial f_{cc}(p_z, z, t)}{\partial z} \\ & + \frac{1}{\hbar} \int dz_1 dp_{z2} \exp\left(\frac{i}{\hbar}z_1(p_z - p_{z2})\right) [E_c(z - \frac{z_1}{2}) - E_c(z + \frac{z_1}{2})] f_{cc}(p_{z2}, z, t) \\ & + \frac{p_z}{m_0} P_{cv} f_{vc}(p_z, z, t) - \frac{i\hbar}{2m_0} P_{cv} \frac{\partial f_{vc}(p_z, z, t)}{\partial z} \\ & + \frac{p_z}{m_0} P_{cv} f_{cv}(p_z, z, t) + \frac{i\hbar}{2m_0} P_{cv} \frac{\partial f_{cv}(p_z, z, t)}{\partial z}, \end{aligned} \quad (47)$$

$$\begin{aligned} i\hbar \frac{\partial f_{cv}(p_z, z, t)}{\partial t} = & -\frac{i\hbar p_z}{m_0} \frac{\partial f_{cv}(p_z, z, t)}{\partial z} \\ & + \frac{1}{\hbar} \int dz_1 dp_{z2} \exp\left(\frac{i}{\hbar}z_1(p_z - p_{z2})\right) [E_c(z - \frac{z_1}{2}) - E_v(z + \frac{z_1}{2})] f_{cv}(p_{z2}, z, t) \\ & + \frac{p_z}{m_0} P_{cv} f_{vv}(p_z, z, t) - \frac{i\hbar}{2m_0} P_{cv} \frac{\partial f_{vv}(p_z, z, t)}{\partial z} \\ & + \frac{p_z}{m_0} P_{cv} f_{cc}(p_z, z, t) - \frac{i\hbar}{2m_0} P_{cv} \frac{\partial f_{cc}(p_z, z, t)}{\partial z}, \end{aligned} \quad (48)$$

$$\begin{aligned} i\hbar \frac{\partial f_{vv}(p_z, z, t)}{\partial t} = & -\frac{i\hbar p_z}{m_0} \frac{\partial f_{vv}(p_z, z, t)}{\partial z} \\ & + \frac{1}{\hbar} \int dz_1 dp_{z2} \exp\left(\frac{i}{\hbar}z_1(p_z - p_{z2})\right) [E_v(z - \frac{z_1}{2}) - E_v(z + \frac{z_1}{2})] f_{vv}(p_{z2}, z, t) \\ & - \frac{p_z}{m_0} P_{cv} f_{cv}(p_z, z, t) + \frac{i\hbar}{2m_0} P_{cv} \frac{\partial f_{cv}(p_z, z, t)}{\partial z} \\ & - \frac{p_z}{m_0} P_{cv} f_{vc}(p_z, z, t) - \frac{i\hbar}{2m_0} P_{cv} \frac{\partial f_{vc}(p_z, z, t)}{\partial z}, \end{aligned} \quad (49)$$

and  $f_{vc} = f_{cv}^*$ . Note that above equations are for the conduction and valence band electrons and  $E_a(z) = E_a(0) + V_a(z)$ . The current density can be calculated using the equation (40) and given by

$$J = J_{intra} + J_{inter} = \frac{e}{\hbar} \int dp_z \frac{p_z}{m_0} (f_{cc}(p_z) + f_{vv}(p_z)) + \frac{2e}{\hbar} \int dp_z \sqrt{\frac{m_0 E_p}{2}} \frac{1}{m_0} \text{Im}[f_{cv}(p_z)]. \quad (50)$$

where  $\text{Im}[f_{cv}]$  means the imaginary part of  $f_{cv}$ . The particle densities in each band using the equation (41) are

$$n_c = \frac{1}{\hbar} \int dp_z f_{cc}(p_z), \quad (51)$$

$$n_v = \frac{1}{\hbar} \int dp_z f_{vv}(p_z). \quad (52)$$

## 4 Conclusions

In this paper we developed multi-band Wigner function formalism including spin, which has a profound effect especially in narrow band-gap semiconductors. We employed the  $\mathbf{k} \cdot \mathbf{p}$  Hamiltonian to derive the quantum transport equations for multi-band semiconductors using non-equilibrium Green's function methodology for systems weakly coupled to a phonon bath. It was shown that in addition to drift, potential and scattering terms that exist in single-band form of Wigner function, there are terms arising from inter-band coupling and spin-orbit interaction. These terms are source of the off-diagonal terms of Wigner function in energy band space and spin space.

A two-band Kane model of resonant inter-band tunneling diode was presented. The current and particle densities were derived for this simple model. We are going to discuss the numerical solution of the two-band and the three-band equations and present the simulation results in future papers.

## 5 Acknowledgments

This work was supported by a grant from the Army Research Office's Defense University Research Initiative on Nanotechnology (DURINT). We thank Greg Recine, Robert Murawski, and Vadim Puller for helpful discussions.

## References

- [1] H. Haug and A. Jauho, *Quantum Kinetics in Transport and Optics of Semiconductors* (Springer, 1996).
- [2] F. A. Buot and K. L. Jensen, *Phys. Rev. B*, 42, 9429, (1990).
- [3] D. Woolard, W. Zhang, B. Gelmont, *Proc. of International Semiconductor Device Research Symposium*, December 10-12, 2003.
- [4] B. Gelmont, D. Woolard, W. Zhang, T. Globus, *Solid State Electronics*, 46, 1513, (2002).
- [5] E. O. Kane, in *Physics of III-V Compounds, Semiconductors and Semimetals*, Vol. 1, 75, (Academic Press, 1966).

- [6] L. P. Kadanoff and G. Baym, Quantum Statistical Mechanics, (Benjamin, 1962).
- [7] F. A. Buot, J. of Stat. Phys., 61, 1223, (1990).
- [8] D. R. Miller and D. P. Neikirk, Appl. Phys. Lett., 58, 2803, (1994).
- [9] L. Demeio, L. Barletti, P. Bordone and C. Jacoboni, Wigner function for multiband transport in semiconductors, Transport Theory and Statistical Physics, 32 (3-4), 321-339 (2003).
- [10] L. Demeio, P. Bordone and C. Jacoboni, Numerical and analytical applications of multiband transport in semiconductors, Proc. XXIII Symposium on Rarefied Gas Dynamics, Whistler, BC, Canada, July 20-25, 2002.
- [11] P. Zhao, N. J. M. Horing and H. L. Cui, Phil. Mag. B, 80, 1359, (2000).
- [12] G. Borgioli, G. Frosali, P. F. Zweifel, Transport Theory Stat. Phys. 32, (2003).
- [13] W. W. Chow and S. W. Koch, Semiconductor-Laser Fundamentals: Physics of the Gain Materials (Springer Verlag, 1999).
- [14] F. A. Buot, Superlattices and Microstructures, 11, 103, (1992).
- [15] F. A. Buot, Phys. Rev. B, 10, 3700, (1974).
- [16] R. F. O'Connell and E. P. Wigner, Phys. Rev. A, 30, 2613, (1984).
- [17] G. D. Mahan, Physics Reports, 145, 251, (1987).
- [18] R. Binder and S. W. Koch, Prog. Quant. Electr., 19, 307, (1995).
- [19] D. Z.-Y. Ting and X. Cartoxia, Appl. Phys. Lett., 81, 4198, (2002).
- [20] T. Koga, J. Nitta, H. Takayanagi and S. Datta, Phys. Rev. Lett., 88, 126601, (2002).
- [21] M. Sweeny and J. Xu, Appl. Phys. Lett., 54, 546, (1989).
- [22] G. Bastard, Wave Mechanics Applied to Semiconductor Heterostructures (Les Editions de Physique, 1988).
- [23] C. Sirtori, F. Capasso and J. Faist, Phys. Rev. B, 50, 8663, (1994).